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Frenkel excitons and band structure in Sb₂S₃ single crystals

Abstract:

Anisotropy of optical properties of Sb₂S₃ single crystals was investigated at 11 and 300 K. Ground and excited states of four excitonic states (*A*, *B*, *C* and *D*) were found out. Parameters of observed excitons and bands *V*₁ – *V*₄ were determined. In Γ point of Brillouin zone the effective masses of electrons in the bottom conduction band ($m_{c^*} = 1.08m_0$) and of holes in four top valence bands (mv_1^* , $mv_2^* = 2.91m_0$ and mv_3^* , $mv_4^* = 3.12m_0$) were estimated. The splitting magnitudes of valence bands *V*₁ – *V*₂ in the Brillouin zone center by crystal field ($\Delta_{cf} = 20$ meV) and by spin-orbital interaction ($\Delta_{so} = 375$ meV) were calculated. *V*₃ and *V*₄ bands have splitting of 198 meV. The observed features

were interpreted on the base of existing theoretically calculated band structure and symmetries of excitons in Γ point of Brillouin zone for single crystals of orthorhombic symmetry (*Pnma*).